(1)

FINAL REPORT

Grant No. N00014-90-J-1731

G. Stell

STUDIES IN CLUSTERING THEORY

1990 ONR

In recent years the properties of percolation models have been studied intensively. These investigations have usually been confined to the study of idealized lattice models, and have generally limited themslves to obtaining the critical exponents and other "universal" data. The purpose of our project was to develop a general theory of percolation and clustering between particles of arbitrary size and shape, with arbitrary correlations between them. The goal of such a theory includes the treatment of continuum percolation as well as a novel treatment of lattice percolation. We made substantial progress toward this goal.[1-5]

The quantities basic to a description of clustering, the mean cluster size, mean number of clusters, etc. were developed[1], in the general case, in terms of a power series in particle density. We gave concise formulas for the terms in such series, and proved[2], at least for sufficiently low densities, that the series are absolutely convergent. These series can now be used to construct Padé approximants that will allow one to probe the percolation transition.

A scaled-particle theory of percolation was developed[3] which gives analytic approximants for the mean number of clusters in a large class of two and three dimensional percolation models. Although this quantity is essential in many applications, e.g., explaining colligative properties, and interpreting low-angle light-scattering data, no systematic studies of it have been done before this work. We recently carried out detailed computer simulations[4] that show that the mean number of clusters is given to high accuracy by several of our approximations. Extensions of this work will allow calculation of the complete cluster size distribution. This work should be of practical importance in studying systems ranging from colloidal dispersions to nano-scale metal clusters.

STONY BROOK

State University of New York

George Stell
Department of Chemistry
State University of New York
Stony Brook, New York 11794-3400
[516] 632-7899/7901
BITNET GSTELL@SBCCMAIL
FAX (516) 632-7960

28 December 1990

Scientific Officer Code: 1112AI
Peter J. Reynolds -696-4205
Office of Naval Research
800 North Quincy Street
Arlington, Virginia 22217-5000

Administrative Grants Officer
Office of Naval Research
Resident Representative N62927
Administrative Contracting Officer
33 Third Avenue - Lower Level
New York, N.Y. 10003-9998

dist. A 1/14/91

Director, Naval Research Laboratory
Attn: Code 2627
Washington, D.C. 20375

Defense Technical Information Center
Building 5, Cameron Station
Alexandria, Virginia 22314

Re.: Grant No. N00014-90-J-1731
PI: George Stell

Dear Sir/Madam:

This material should have accompanied our Report Documentation Page, but appears not to have.

Sincerely yours,

George Stell

George Stell
Leading Professor of
Chemistry and Mechanical
Engineering

GS/is
Encl.

We found, as we had hoped, that our general formalism leads to novel and effective approximation schemes for lattice-percolation problems as well as continuum-percolation problems, and we have summarized our results in this direction in a paper[5] that will appear in J. Phys. A. They lead to a new method of approximating the pair connectedness function for bond percolation problems.

A ubiquitious feature of physical clustering in a wide variety of random materials is the size polydispersity of the elements or grains that constitute the materials. We have developed a powerful approximation method to characterize with high accuracy the microstructure of such polydisperse material and have applied it to two important porous-media problems for polydisperse media — the determination of permeability[6] to fluid flow in such media and the determination of trapping rates[7] for diffusion-controlled reactions in a fluid diffusing through such a medium that reacts with the fluid. Out new results include assessments of permeability and trapping rate that constitute an upper bound on permeabilities and a lower bound on trapping rates that are sharp (i.e., exact) in the limit of high porosity (i.e., vanishingly low volume fraction of medium).

References

[1] J. A. Given and G. Stell, "The Continuum Potts Model and Continuum Percolation", Physica A **161**, 152-180 (1989)

[2] J. A. Given and G. Stell, "The Kirkwood-Salsburg Equations for Random Continuum Percolation", J. Stat. Phys. **59**, 981-1018 (1990)

[3] J. A. Given and G. Stell, "Scaled-Particle Theory and the Short-Distance Behavior of Continuum Percolation", J. Chem. Phys. **92**, 4433-4446 (1990)

[4] J.A. Given, I.C. Chan, S. Torquato, and G. Stell, "Comparison of Analytic and Numerical Results for the Mean Cluster Density in Continuum Percolation", J. Chem. Phys. **93**, 5128-5139 (1990)

[5] J.A. Given and G. Stell, "Approximations of Mean Spherical Type for Lattice Percolation Models", (accepted for publication, J. Phys. A)

[6] J.A. Given and G. Stell, "Improved Permeability Bounds for Highly Polydisperse Materials", Phys. Fluids A **2**, 1929-1936 (1990).

[7] J.A. Given, J. Blawzdziewicz, and G. Stell, "Diffusion-controlled Reactions in a Polydisperse Medium of Reactive Sinks", J. Chem. Phys. **93**, 8156-8169 (1990).